ESRF	**Experiment title:** STRUCTURAL DETERMINATION OF THE Si/Cu(110) INTERFACE	**Experiment number:** SI-221
Beamline: ID-03	**Date of experiment:** from: 12-8-96 to: 20-8-96	**Date of report:** Aug.96
Shifts: 18	**Local contact(s):** X. Torrellas	*Received at ESRF:*

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Report:

18 shifts were allocated in the beam line ID-3 (Surface Diffraction-proposal SI-221) in August-96 to resolve the atomic structure of the Si/Cu(110) interface.

The objective of the proposal was twofold. The First goal was to discern between two different atomic models suggested by previous photoelectron diffraction experiments, and secondly, to give accurate values for the atomic positions of the correct model.

Sample preparation was done by following the standard procedure used in our home laboratory. This procedure leads to high quality LEED patterns on the substrate that was used at the ESRF for experiments. However, the sample resulted to be of a poor quality for the X-Ray Surface Diffraction due to the high surface and bulk sensitivity over the whole sample of this technique. This fact was evidenced by measuring the width of the CTR minimum which indicated a width of the atomically ordered terraces of around 250 $Å^2$.

In addition to that, the single Cu(110) crystal contained other little crystallite misoriented with respect to the main one, which presented some extra Brag peaks and Thermal Diffuse Scattering background at specific points of the reciprocal space.

Experiments were performed with the two previously described backdraws. Thus, Si was deposited to form the c(2x2) superstructure and Fractionary order diffraction peaks were detected. The width of these peaks suggested that the ordered terrace's width was around 50 A'.

Nevertheless and because of the high flux of the ESRF a set of in-plane reflections could be measured (see figure 1). In addition to those, fractional order rods and CTR were also recorded (see fig. 2a and 2b, respectively). The quality of the data was limited by the unusual background induced by the second crystallite and by the width of the diffraction peaks induced by the bad crystal quality.

Although the big error bar, the integrated intensity of the in-plane reflections has allowed us to discern between the different proposed geometrical models for the superstructure (first objective of the proposal). Thus, the actual in-plane atomic model consists of Si atoms replacing substitutionaly Cu atoms in the (110) surface rows, forming a surface alloy. However, the vertical displacement between Si and Cu atoms at the surface layer has not been found. Although modulation in the Si modified CTRs has been observed, the differences between equivalent CTR induced by the background disable an accurate fit of the data.

All these findings are uncompleted and then, a new set of experiments using a single crystal of better quality and the experience acquired in this beam time, would be essential.